

Diethyl sulfate

64-67-5 | DTXSID1024045

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	1.14	0.85	1.12	0.83	1.23

Model Results

Predicted value: $1.55\text{e-}12 \text{ cm}^3/\text{molecule}\cdot\text{sec}$

Global applicability domain: Inside

Local applicability domain index: $4.02\text{e-}01$

Confidence level: $8.17\text{e-}01$

Nearest Neighbors from the Training Set

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Diethyl sulfate

Measured: $1.80\text{e-}12$

Predicted: $1.55\text{e-}12$

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Dimethyl sulfate

Measured: $5.00\text{e-}13$

Predicted: $4.96\text{e-}13$

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Isobutyl nitrate

Measured: $9.20\text{e-}13$

Predicted: $1.33\text{e-}12$

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Butyl nitrate

Measured: $1.71\text{e-}12$

Predicted: $1.60\text{e-}12$

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n-Propyl nitrate

Measured: $7.30\text{e-}13$

Predicted: $8.54\text{e-}13$